Morphology and charging of heteropolar SiC/AlN and SiC/GaN interfaces

Małgorzata Sznajder[1] **and Jacek A. Majewski**[2]

[1] *Institute of Physics, University of Rzeszów, ul. Rejtana 16a, 35-310 Rzeszów, Poland*
[2] *Faculty of Physics, University of Warsaw, ul. Hoża 69, 00-681 Warszawa, Poland*

Thin nitride films on silicon carbide substrate constitute many technologically important devices [1,2], where the nitride/SiC interface plays particularly important role. In spite of intensive experimental efforts [e.g., 3], the microscopic physics of these intriguing interfaces is mostly unknown. The heterovalent character of these interfaces, in addition to the piezo- and pyroelectric character of the junction materials, leads to polarization charges and very strong electric fields that could in turn cause changes in atomistic details of the interfaces.

In this work, we present first-principles studies for 4H-SiC/wz-AlN, 3C-SiC(111)/wz-AlN, 4H-SiC/wz-GaN, and 3C-SiC/wz-GaN interfaces in the framework of the density functional theory. We have calculated the atomistic details of the interfaces, their formation enthalpies, valence band offsets (VBO's), induced interface charges, and electric fields. The theoretical studies of the similar interfaces have been reported previously for some cubic structures [4]. In the present calculations we employed the supercells with up to 136 atoms, and performed precise calculations for hexagonal systems employing the SIESTA code.

In heteropolar SiC/nitride systems, the abrupt interfaces contain 'oversaturated' or 'under saturated ' tetrahedral bonds with more than 2 or less than 2 electrons per bond, respectively. This bond heteropolarity leads to a macroscopically charged interface that is typically energetically unstable and undergoes various reconstructions to roughly restore charge neutrality. For example, the simplest atomic reconstructions leading to the neutral interfaces are those with one mixed layer (e.g., N/C, Ga/Si or Al/Si).

Our calculations show that the preferred bonding configurations of the reconstructed interfaces are found to be Si-N and Ga-C. The calculated valence band discontinuities for SiC/AlN and SiC/GaN heterostructures lie in the range of 1.5 - 2.3 eV and 0.4 - 1.4 eV, respectively, depending on the atomistic details of the reconstruction, and compare reasonably well with available experimental data. The SiC/AlN heterostructures are predicted to be of type I, whereas SiC/GaN heterostructures can be of type I or II, depending on the orientation and chemical composition of the interface. The polarization induced interface charges are of the order of 4.8 x 10^{12}cm^{-2} and 0.7 x 10^{12} cm^{-2} in SiC/AlN and SiC/GaN junctions, respectively. Comparing the interface charges in the junctions with hexagonal 4H-SiC and cubic 3C-SiC heterostructures, we conclude that the spontaneous polarization in bulk 4H-SiC is negligible in comparison to the one in AlN and GaN.

The present studies shed light on the physics of heteropolar SiC/nitride interfaces and provide microscopic knowledge of interface morphology together with theoretical predictions of important parameters of the junctions. They constitute also the basis for reliable modeling of important phenomena in these junctions such as the charge and spin transport across the interface and the thermal boundary resistance effect.

[1] A. V. Sampath, *et al*., Appl. Phys. Lett. **101**, 093506 (2012).
[2] Y. Huang, *et al*., Appl. Phys. Lett. **86**, 122102 (2005).
[3] S. W. King, R. F. Davis, and R. J. Nemanich, Surf. Sci. **602**, 405 (2008); M. Losurdo, *et al*., Appl. Phys. Lett. **86**, 021920 (2005).
[4] M. Städele, J.A. Majewski, and P. Vogl, Phys. Rev. B **56**, 6911 (1997); P. Ferrara, N. Binggeli, and A. Baldereschi, Phys. Rev. B **55**, R7418 (1997).